Supporting information for

Enhanced Gas Separation Properties of Tröger's Base Polymer Membranes Derived from Pure Triptycene Diamine Regioisomers

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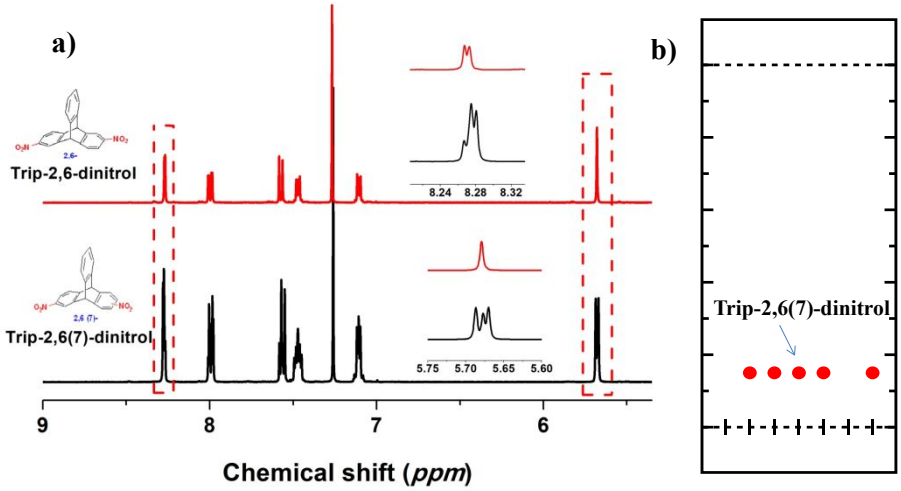

Figure S1. a) NMR spectra of Trip-2,6-dinitrol and mixture of Trip-2,6(7)-dinitrol, the bridge head proton ~ 5.7 ppm and proton in the ortho position of nitrol group ~ 8.28 ppm was highlighted on the magnified NMR spectra; b) Thin layer chromatography (TLC) point of Trip- 2,6(7)-dinitrol mixed compound, the eluent is dichloromethane/petroleum ether =1/3, R_f = 0.15.

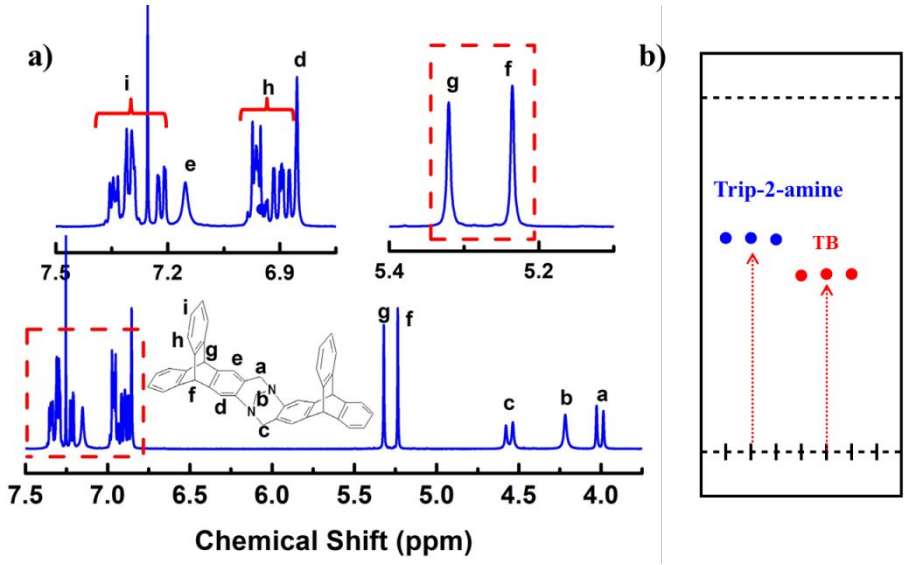

Figure S2. a) NMR spectra of model compound triptycene-TB, the bridge head protons ~ 5.3 ppm and aromatic protons ~ 6.9 to 7.3 ppm are highlighted in the magnified figure. b) TLC of the reaction with eluent of dichloromethane/ethyl acetate = 4/1; R_f = 0.5 (red), R_f of the starting material is 0.6 (blue).

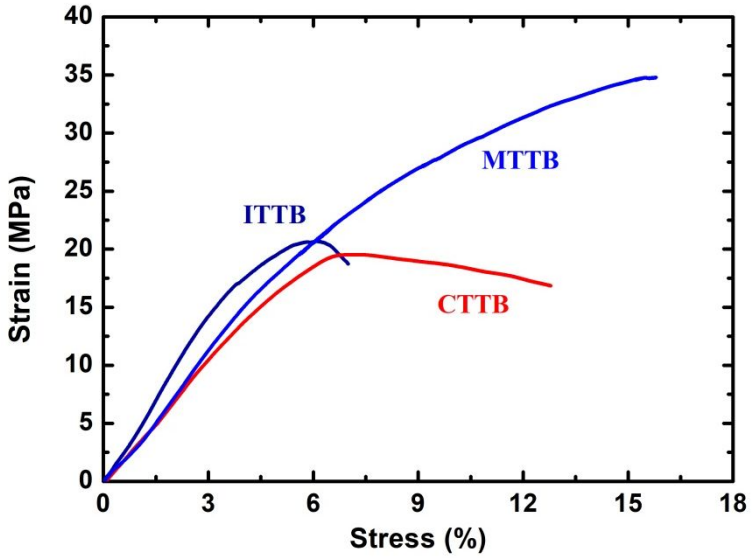

Figure S3. Stress-strain curves of CTTB, ITTB and MTTB, all polymers were fresh made by soaking in MeOH for 12 h and then air-dried for 3 days.

Table S1. Mechanical Properties of the ITTB, CTTB and MTTB Polymer Membranes

Polymers	Young's Modulus (GPa)	Strain (Mpa)	Elongation at break %	yielding
ITTB	0.50	20	6%	Yes (at 5.8%)
CTTB	0.42	18	13%	Yes (at 6.2%)
MTTB	0.44	35	17%	No

Young's Modulus is obtained from the Stress-Strain curve in the strain range between 5 to 10 Mpa.

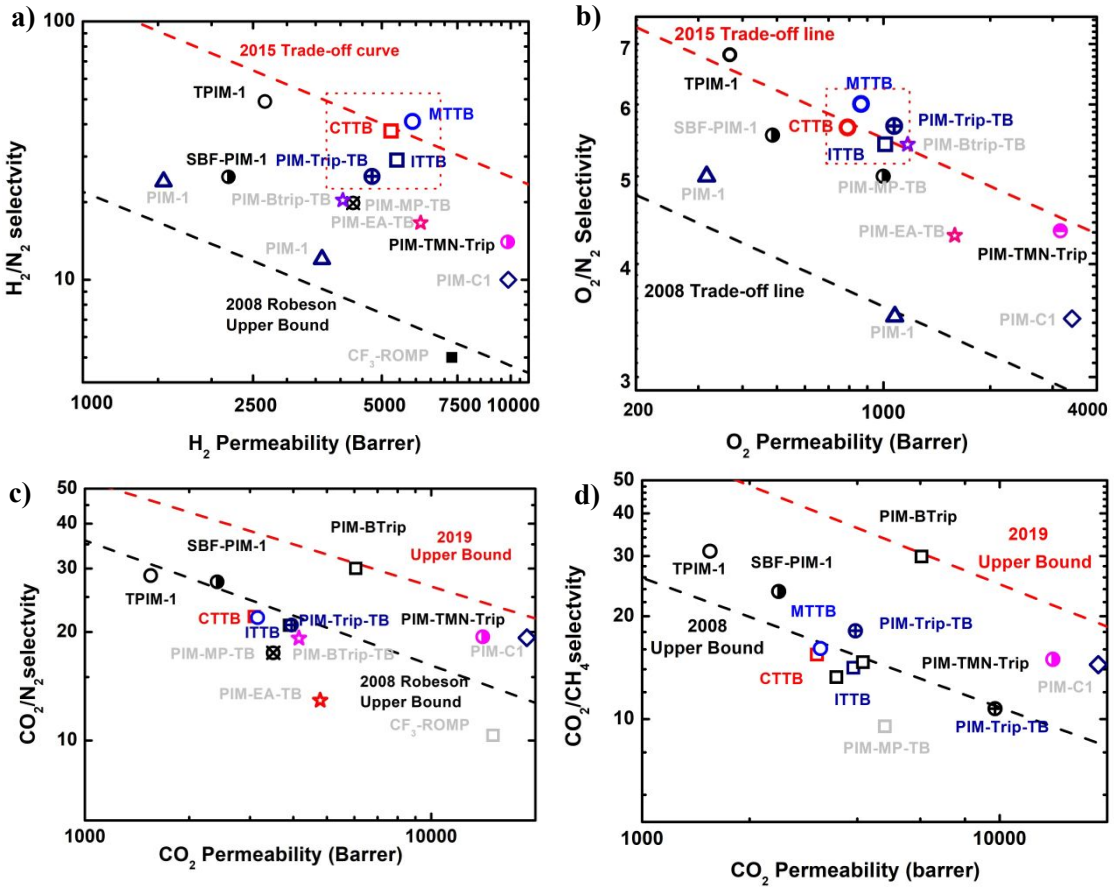

Figure S4. H_2/N_2 (a) and O_2/N_2 (b) CO_2/N_2 (c) and CO_2/CH_4 (d) separation performance of CTTB, MTTB, ITTB and some other reported polymers.

Table S2. Diffusivity and Solubility Coefficient of the Polymers Membranes

Polymers	Diffusion coefficient		Solubility coefficient		D_{O2}/D_{N2}	S_{O2}/S_{N2}
	N_2	O_2	N_2	O_2		
CTTB[a]	20.5	106	6.85	7.49	5.17	1.09
MTTB[b]	20.1	110	7.14	7.87	5.47	1.10
ITTB[c]	22.4	115	8.35	8.8	5.13	1.05

[a]CTTB with the thickness of 54 μm, fresh air-dried membrane. [b]MTTB with the thickness of 60 μm, fresh air-dried membrane. [c]ITTB with the thickness of 54 μm, fresh air-dried membranes.

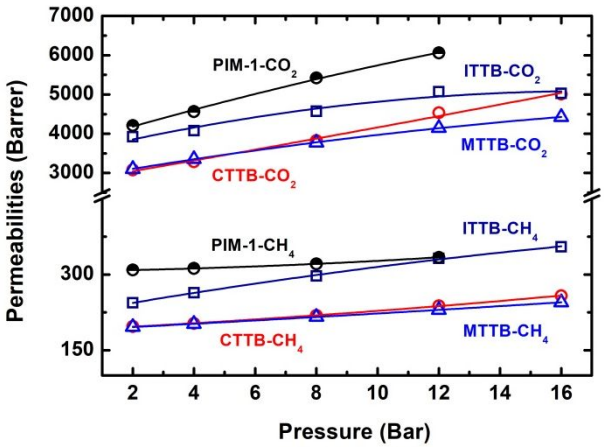

Figure S5: Pressure dependence of CO_2 and CH_4 permeabilities for CTTB, MTTB, ITTB and PIM-1.

Table S3. CO_2 and CH_4 Pressure Dependence of CTTB, MTTB, ITTB and PIM-1

Permeability (Barrer)		2 Bar	4 Bar	8 Bar	12 Bar	16 Bar
CTTB	P_{CH4}	197	203	219	238	258
	P_{CO2}	3080	3284	3821	4535	5008
	P_{CO2}/P_{CH4}	15.6	16.2	17.4	19.0	19.4
MTTB	P_{CH4}	196	202	216	230	245
	P_{CO2}	3101	3356	3772	4146	4427
	P_{CO2}/P_{CH4}	15.8	16.6	17.4	18.0	18.1
ITTB	P_{CH4}	244	264	297	332	355
	P_{CO2}	3923	4078	4573	5074	5031
	P_{CO2}/P_{CH4}	16.1	15.4	15.4	15.3	14.2
PIM-1	P_{CH4}	309	312	321	334	
	P_{CO2}	4208	4563	5421	6060	
	P_{CO2}/P_{CH4}	13.6	14.6	16.9	18.1	

The thickness of the above membranes was ~ 60 μm and the polymer membranes were soaked in methanol for 12h and then air-dried for 3 days before testing.

Table S4. Activation Energy of the CTTB, MTTB and ITTB for O_2 and N_2.

Polymer		Slop	R^2	ΔE_P (Kcal/mol)
CTTB [a]	O_2	-0.94	0.975	0.0575
	N_2	-1.33	0.973	0.0814
MTTB [b]	O_2	-1.21	0.996	0.0740
	N_2	-1.93	0.983	0.1181
ITTB [c]	O_2	-0.66	0.997	0.0404
	N_2	-0.84	0.998	0.0513

[a]CTTB with the thickness of 54 μm, fresh air-dried membrane. [b]MTTB with the thickness of 60 μm, fresh air-dried membrane. [c]ITTB with the thickness of 54 μm, fresh air-dried membranes.